

**HYDROGEN AND HELIUM BROADENING AND PRESSURE INDUCED LINE SHIFTS
OF $^{13}\text{CH}_4$ IN THE ν_4 BAND**

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ABSTRACT

Hydrogen and helium pressure induced broadening and line shifts of the ν_4 band of isotopic methane ($^{13}\text{CH}_4$) have been measured at room temperature for many lines in the P, Q and R branches. The measurements were obtained using the one meter Fourier Transform Spectrometer at the KPNO McMath Solar Telescope with a spectral resolution of 0.0065 cm^{-1} . Data were obtained for 266 absorption lines for a range of J values up to $J = 16$; the pressure broadening results are compared to similar measurements made for the common isotope $^{12}\text{CH}_4$ and a small, but consistent variation is noted.

INTRODUCTION. In an earlier work the broadening of methane $^{12}\text{CH}_4$ lines by hydrogen at two separate temperatures for the ν_4 band was reported¹. In studies of methane broadening by some other gases it has been noted that there are differences in the broadening parameters for the two common carbon isotopes^{2,3,4,5}. In this work we report on the pressure broadening and shifts of some lines in the ν_4 band of the $^{13}\text{CH}_4$ isotopomer; the broadeners are hydrogen and helium and all measurements are made at room temperature. It is expected that these results will find application in the analysis of the observations of methane in the spectra of the atmospheres of the outer planets; methane gas is a major contributor to the optical opacity of the atmospheres of those planets, which have mainly hydrogen and helium atmospheres. It is known from previous studies that the appearance of atmospheric spectra are sensitive to the values of the broadening parameters of the absorption lines (Gibson and Pierluissi)⁶. For example, Smith and Gordley⁷ have pointed out that the use of inaccurate widths can lead to significant errors in the retrieved profiles of ozone in the earth's atmosphere for broad-band radiometric data or for isolated strong lines observed in high-resolution spectra. Unfortunately, there does not seem to be a corresponding study of the sensitivity of retrievals of atmospheric parameters for hydrogen broadened methane atmospheres; however, there is no reason to believe that retrievals of atmospheric parameters using methane lines would be any less sensitive to errors in the methane parameters than for the corresponding ozone parameters. Also, there does not appear to be any studies of the effects on retrievals due to ignoring the pressure shifts in atmospheric spectra. Nevertheless, these parameters are presented here.

Many studies of the broadening of $^{12}\text{CH}_4$ have been made considering self-broadening (Ballard and Johnston)⁸; air, nitrogen and oxygen broadeners by the Langley Research Center investigators^{9,10} and Fox et al¹¹ and others. The number of studies of pressure induced shifts is sparse; this parameter is somewhat more difficult to measure than either line intensities or widths and may be somewhat less important in the quantitative analysis of spectra depending on the type of observation and the magnitude of the shift. The study by Malathy Devi et al¹² for the ν_3 band of methane demonstrates that the pressure shifts for methane lines may be as large as 20% or more of the pressure broadening. Also, although there appears to be a reasonable correlation of broadening coefficients between bands and even isotopomers, the pressure induced shifts seem to have no correlation with each other from band to band. For example, the shifts for corresponding quantum numbers for the ^{13}C isotopomer for the methane ν_4 and ν_3 bands, as measured by Malathy Devi et al.^{2,3} do not agree well with each although the widths corresponding to the same quantum numbers do. There does appear to be some indication that there is a tendency for the pressure shifts to increase with increasing frequency.

EXPERIMENTAL. The spectra for this study were obtained using the one meter Fourier Transform Spectrometer at the McMath Solar Telescope (Kitt Peak National Observatory) with a spectral resolution of 0.0065 cm^{-1} (full width at half maximum). They were all acquired at room temperature (296K) using 99.5% pure isotopic ^{13}C methane in either a 25 or 150 cm cell. CO, which was contained in a separate external at low pressure, cell was used to establish a frequency calibration for each spectrum used for the determination of the pressure shift. For the pressure shift determination it is not necessary, in fact, to have an absolute frequency standard; a relative standard suffices provided that the zero pressure line position is not obtained from, for example, the HITRAN¹³ line list, but is separately determined. The conditions of pressure and path-length for this study are listed in table 1. All pressures were measured by using a temperature compensated capacitance type manometer manufactured by MKS Baratron. The values shown for the methane pressures are not exact and should be regarded as nominal; the methane is introduced into the cell before introducing the pressurizing gas. What happens to the methane gas partial pressure after admitting the pressurizing gas is uncertain and not of much importance to the determination of the broadening coefficient so long as it does not increase to the point that self-broadening becomes important. These conditions allowed a range of absorption strengths of approximately 2.75×10^{-24} to $1.0 \times 10^{-21}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$ (in HITRAN¹³ units, which assumes a normal isotopic abundance for the ^{13}C isotope) to be measured. In all, measurements of 266 lines are reported, As in previous studies at this laboratory by the author the data were analyzed using a method of least squares which fits a synthetic spectrum based on a Voigt line-shape and semi-empirically determined instrumental line-shape to each of the absorption lines identified in the spectra¹⁴ (for a small number, less than about 12, of lines at a time). The values reported for the pressure broadening were obtained by averaging the individual pressure broadening coefficients, determined separately from the spectra; the uncertainties reported with the broadening and shift values are the RMS variations of the averages of the individual values and do not represent the complete error budget. The pressure induced shift was determined by fitting a straight line to the individual line centers for the different pressure conditions. A low pressure methane spectrum, not pressurized by a foreign gas, was also calibrated and measured independently instead of relying on the published HITRAN values for the unshifted line centers for the pressure shift determination. The fitting routine assumes a constant value of self-broadening of $0.08\text{ cm}^{-1}/\text{atm}$. The small variations in this value which naturally occur will have little effect on the accuracy of the final result due to the small methane pressures used. For example, a variation of the self-broadening from 0.06 to $0.10\text{ cm}^{-1}/\text{atm}$ would change the measured value by 2% for the worst case, highest methane pressure, narrowest helium broadened lines. For all other cases the effect of self-broadening will be less. Since the broadening coefficient is averaged in with values less sensitive to the self-broadening, the reported values are much less sensitive. For isolated lines it is noted that the least squares retrieved value of the broadening coefficient is somewhat dependent on the way that the calculation is initiated; for example, small variations in the retrieved width are noted depending on the width of the spectral interval used in the calculation and the initial guess at the parameter values. However, the variations noted do not exceed 1%. The pressures are read from a single gauge with an accuracy estimated at about 1 torr. Non-linearities in the IR detector used with the spectrometer will, among other effects, cause the zero signal

level to be displaced from the displayed value. This will affect the apparent line shape, especially for strongly absorbing lines. The retrieved value of the line-width will then be different from the correct value. However, within the range of methane densities used in these measurements there is no consistent variation in retrieved values of the line-width with methane density as would be expected if there were a significant non-linear behavior of the detector system. All instrumental effects for determination of line-width for isolated lines are estimated to cause no more than about 2% uncertainty; the standard deviation of the moderately absorbing isolated line measurements is, indeed, about that amount.

The estimate of the uncertainty in the determination of the pressure shift depends on the uncertainty in determination of the line position. The best case, again, is that of an isolated line. The determination of line position depends on both the width and signal-to-noise ratio in the spectrum as well as the peak depth of the measured line. On average., I estimate that the position of a broadened isolated absorption line could be measured with an uncertainty of 0.0002 cm-l; the unbroadened absorption lines, being much narrower, were measured with greater precision. The accuracy of the pressure shift coefficient then depends on the size of the pressure shift; large pressure shift coefficients being determined more accurately than small coefficients. For large values of the shift coefficient (on the order of 10% of the width coefficient) the uncertainty in the shift coefficient is about 2% and increases inversely proportional to the shift. For blended lines the uncertainties in the measured line positions increase rapidly with the extent of the blending and the uncertainty in the shift coefficient is correspondingly greater than for isolated lines.

Figure 1 shows some examples of a fit to a single isolated helium broadened absorption line. In figure 1a the line position, intensity and width were allowed to vary in obtaining the fit, The random character of the residuals in the plot 1a illustrates the high S/N obtained with the Mcmath FTS. In figure 1b the width was increased by 3% from the value obtained in 1a and then kept fixed; all other parameters were allowed to vary in obtaining a new fit to the data. These two figures demonstrate the significant changes which take place in the residuals with a small change in line-width and can be used to provide a numerical estimate of the sensitivity of the retrieval method and the uncertainty in the retrieved value of this parameter, Figure 2 illustrates an example of a fit to some lines of the R8 manifold broadened by helium at two different pressures. The fit for the low pressure case (2a) produces residuals with about the same amplitude as for the isolated line case; however, (2b), corresponding to significantly higher broadening pressure, exhibits residuals with somewhat larger amplitude, but still with no apparent systematic variation, this provides further confidence that the assumption of the Voigt absorption line-shape is correct.

The measured widths and shifts for H₂ and He are presented in table 2. The line positions given there are taken from the HITRAN 1992 line list¹³. For comparison purposes the results of the H₂ broadened widths of the common isotope ¹²CH₄¹ are shown in the column next to the last. The ratio of widths for the two isotopes, which is on the average 4% greater for the more common isotope, is shown in the last column. The larger broadening parameter for the ¹²CH₄ isotope is similar to what is observed for air broadening There is a fair amount of variation from line to line; it appears that a few lines of the ¹²C isotope have a smaller broadening coefficient than does the ¹³C isotope.

The measured widths are plotted in figure 3 separately for H₂ and He broadeners as a function of rotational quantum number m, defined as -J" for the P-branch, and J" + 1 for the R-branch; the Q-branch is omitted.

DISCUSSION. The dependence of the width parameters on vibrational quantum number appears to be slight. This is indicated by the measurements of air and N₂ broadened methane bands by the Langley and other groups. It also appears to be the case for H₂ broadened ¹²CH₄ as demonstrated by comparison of the v₄¹ and the 4200 cm⁻¹ bands¹⁵. There appears to be very little consistency in the shift parameters from band to band, and, indeed, the shift parameters show no discernible pattern when plotted in a simple manner as a function of rotational quantum number J. As in previous studies of methane broadening the lines of symmetry type E appear to have smaller broadening coefficients than do the lines of the other types.

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Figure 1a. Example of least squares fit and residuals to isolate.d line: P7 F12 at 1253.69279 cm^{-1} as measured with broadening pressure of 244 torr of He and a nominal pressure of 2.7 torr of $^{13}\text{CH}_4$ in a 25 cm cell. The vertical axis is proportional to signal intensity at the detector; the residuals are in percentage of the difference with respect to the continuum level. The chisquare for this fit is 0.000125.

Figure 1b. Example of least squares fit as above except that the pressure broadening coefficient is increased by 3%. The chisquare has increased to 0.000259.

Figure 2. Example of least squares fit to part of the R8 manifold: The main absorption shown are R8 E1 at 1344.16843 cm^{-1} , R8 F1 1 at 1344.21535 cm^{-1} and R8 A1 1 at 1344.29582 cm^{-1} . panel a) corresponds to a broadening pressure of 244 torr of 1 He while b) corresponds to 594 torr. Several weaker features appearing in this spectral interval were included in the fit.

Figure 3a. Measured hydrogen broadened widths for the P- and R-Banches of the ν_4 band of $^{13}\text{CH}_4$. The widths of the five symmetry types are displayed separately.

Figure 3b. Measured helium broadened widths for the P- and R-Banches of the ν_4 band of $^{13}\text{CH}_4$.

Table 2. Measured widths and shifts for hydrogen and helium broadened $^{13}\text{CH}_4$. Line positions are taken from the HITRAN compilation¹³. The last two columns contain results for previously obtained measurements of corresponding $^{12}\text{CH}_4$ lines¹ broadened by hydrogen. The ratio of broadening coefficients is given in the last column. Frequencies are given in cm^{-1} and widths in $\text{cm}^{-1}/\text{atm}(\text{HWHM})$.

TABLE 1. Conditions for spectra used to determine H₂ and He broadening and shifting of the ¹³CH₄ absorpt ion lines. Methane pressures are nominal values.

path length	¹³ CH ₄ pressure	broadener pressure	broadener gas
0.25 m	1.5 torr	254 torr	H ₂
		384	
		504	
		327	
		344	
		563	
		340	
		474	
		602	
		427	
1.50	1.6	562	
		244	He
		364	
		604	
		269	
		393	
		601	
		324	
		441	
		596	
0.25	2.7	320	
		520	
		.	
		.	
		.	
1.50	6.5	324	
		441	
		596	
		320	
		520	
		.	
		.	
		.	
		.	
		.	

Table 2.

frequency	$\gamma^0(^{13}\text{CH}_4:\text{H}_2)$	$\delta^0(^{13}\text{CH}_4:\text{H}_2)$	$\gamma^0(^{13}\text{CH}_4:\text{He})$	$\delta^0(^{13}\text{CH}_4:\text{He})$	J'	Γ^*	N'	J''	Γ''	N''	$\gamma^0(^{12}\text{CH}_4:\text{H}_2)$	ratio
1184.45771	0.0530(14)	-0.0031(13)	0.0320(11)	-0.0013(7)	15 F2 9 16 F1 3							
1185.53872	0.0526(10)	-0.0008(1)	0.0337(13)	-0.0001(4)	14 A1 3 15 A2 2							
1185.61096	0.0570(25)	0.0016(34)	0.0327(21)	-0.0043 [22)	15 F110 16 F2 3							
1186.01256	0.0508(3)	0.0008(4)	0.0314(22)	0.0013(11)	14 F1 8 15 F2 4							
1187.29735	0.0503(12)	-0.0029(2)	0.0340(6)	-0.0012(4)	14 A2 3 15 A1 1							
1189.04765	0.0496(13)	-0.0022(5)	0.0309(15)	-0.0005(15)	15 A1 4 16 A2 1							
1190.16866	0.0476(17)	-0.0006(21)	0.0291(10)	-0.0006(5)	15 Fill 16 F2 2							
1190.31368	0.0447(32)	-0.0021(16)	0.0243(7)	-0.0006(3)	16 A2 4 17 A1 1							
1190.53866	0.0520(33)	-0.0055(34)	0.0307(12)	-0.0004(10)	15 E 716 E 2							
1190.70631	0.0606(12)	-0.0012(8)	0.0362(7)	-0.0031(12)	9 A2 2 10 A1 1							
1193.07281	0.0532 31	-0.0018(7)	0.0336 4	-0.0016(7)	14 F2 9 15 F1 3							
1193.73968	0.0494 20)	-0.0004(15)	0.0281 10)	-0.0006(5)	14 E 6 15 E 2							
1195.45605	0.0538 8)	-0.0007(4)	0.0348 7)	-0.0003(2)	13 F1 7 14 F2 4							
1195.93435	0.0307 6)	0.0012(6)	0.0180 7)	-0.0008(4)	13 E 5 1 4 E 3							
1196.67785	0.0503 6)	0.0003(15)	0.0321 7)	-0.0031(15)	13 F2 8 14 F1 3							
1196.9215?	0.0452 16)	-0.0040(8)	0.0271 6)	-0.0021(8)	15 F210 16 F1 2							
1197.94292	0.0494 8)	-0.0018(15)	0.02961 6)	-0.0008(2)	14 F210 15 F1 2							
1201.74344	0.0537 5)	-0.0026(i)	0.0328 6)	-0.0008(3)	13 F1 8 14 F2 3							
1203.46200	0.0489 8)	-0.0003(19)	0.0289 9)	-0.0006(5)	14 E 7 15 E 1							
1203.56902	0.0491 6)	-0.0018(6)	0.0284 8)	-0.0004(4)	14 F110 15 F2 2							
1253.76342	0.0499 4)	-0.0022(7)	0.0282 6)	-0.0009(1)	14 A1 4 15 A2 1							
1203.92011	0.0503 4)	-0.0030(5)	0.0293 3)	-0.0012(3)	13 E 614 E 2							
1204.59689	0.0536 7)	-0.0020(4)	0.0324 5)	-0.0010(2)	13 F2 9 14 F1 2	0.0538(7)	1.0037					
1204.77241	0.0542 5)	-0.0016(5)	0.0344(7)	-0.0003(3)	12 F2 7 13 F1 4	0.0558(10)	1.0295					
1205.39414	0.0318(3)	-0.0029(2)	0.0185(3)	-0.0008(2)	12 E 513 E 2	0.0331(13)	1.0409					
1206.02502	0.0535(8)	-0.0044(5)	0.0347(7)	-0.0018(2)	12 F1 7 13 F2 3	0.0547(16)	1.0224					
1209.95270	0.0539(7)	-0.0031(5)	0.0330(5)	-0.0017(3)	12 A1 3 13 A2 1	0.0584(19)	1.0835					
1209.98066	0.0531(13)	-0.0022(13)	0.0322(6)	-0.0007(5)	13 F210 14 F1 1							
1210.27012	0.0494(10)	'0.0020(7)	0.0294(5)	-0.0006(3)	13 F1 9 14 F2 2							
1211.33336	9.0556! 7)	-0.0023(2)	0.0347(6)	-0.0008(2)	12 F1 8 13 F2 2	0.0579(19)	1.0414					
1211.54999	0.0425(19)	-0.0016(12)	0.0225(9)	0.0010(15)	14 Fill 15 F2 1							
1211.56234	0.0412(25)	-0.0028(19)	0.0223(7)	0.0002(10)	14 F211 15 F1 1							
1212.29308	0.0565(5)	-0.0037(2)	0.0337(10)	-0.0014(3)	12 F2 8 13 F1 3	0.0547(23)	0.9681					
1213.54178	0.0561(4)	-0.0011(2)	0.0357(2)	-0.0003(2)	11 A2 2 12 A1 2	0.0585(4)	1.0428					
1214.05163	0.0548(5)	0.0004(8)	0.0354(3)	-0.0002(3)	11 F2 6 12 F1 3	0.0586(18)	1.0693					
1214.68452	0.0562(7)	-0.0046(4)	0.0354(2)	-0.0022(2)	11 F1 7 12 F2 3	0.0586(11)	1.0427					
1215.66064	0.0552(4)	-0.0024(2)	0.0350(2)	-0.0010(2)	11 A1 3 12 A2 1	0.0567(17)	1.0272					
1216.19130	0.0535(5)	-0.0038(4)	0.0326(2)	-0.0014(2)	12 A2 3 13 A1 1	0.0547(12)	1.0224					
1216.68156	0.0527(5)	-0.0023(3)	0.0315(2)	-0.0007(3)	12 F2 9 13 F1 2	0.0529(24)	1.0038					
1216.87377	0.0518(7)	-0.0014(4)	0.0302(7)	-0.0006(2)	12 E 613 E 2	0.0538(6)	1.0386					
1217.42655	0.0453(9)	-0.0027(15)	0.0248(3)	-0.0004(4)	13 A1 3 14 A2 1							
1217.44772	0.0483(33)	-0.0024(16)	0.0262(7)	0.0014(16)	13 F110 14 F2 1							
1219.08308	0.0558(5)	-0.0025(1)	0.0346(5)	-0.0010(2)	11 F1 8 12 F2 2	0.0591 25)	1.0591					
1219.60894	0.0542(6)	-0.0010(3)	0.0324(6)	-0.0005(3)	11 E 512 E 2	0.0547 12)	1.0092					
1220.95865	0.0694(4)	-0.0027(16)	0.0422(15)	-0.0006(10)	6 A1 1 7 A2 1							
1222.45313	0.0570(6)	-0.0007(4)	0.0364(2)	0.0000(2)	10 F2 6 11 F1 3	0.0578 21)	1.0140					
1222.87841	0.0541(13)	-0.0033(5)	0.0336(3)	-0.0010(2)	11 F2 7 12 F1 2							

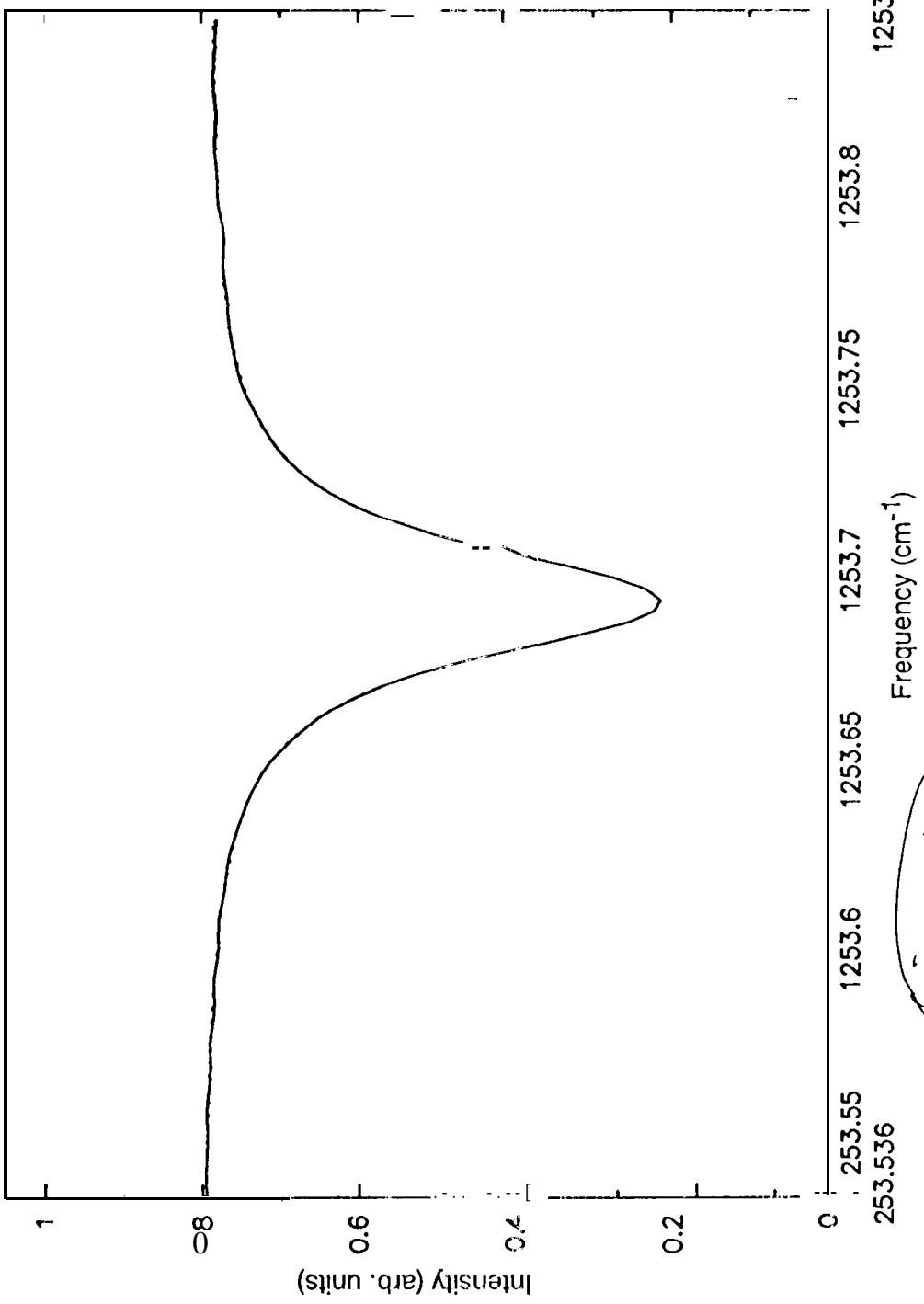
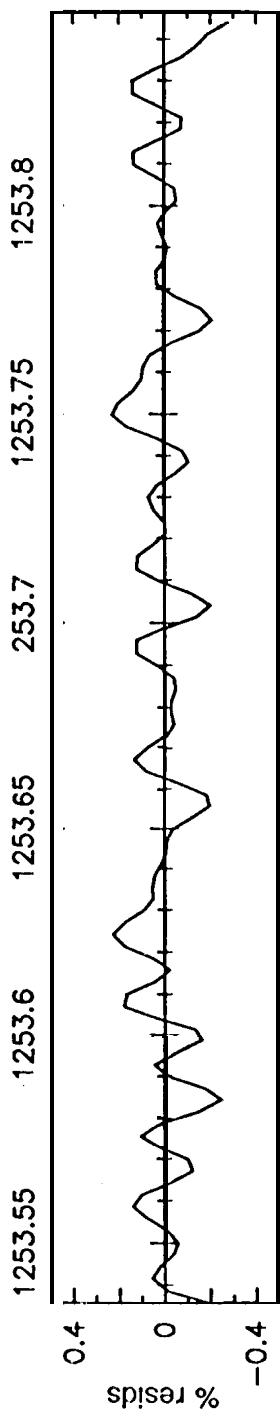
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1223.30517	0.0450(7)	-0.0037(9)	0.0262(5)	-0.0015(3)	12 F1 9 13 F2 1	0.0453(20)	1.0067
1223.33957	0.0542(10)	-0.0028(5)	0.0279(5)	0.0000(3)	12 F210 13 F1 1		
1223.47662	0.0553(7)	-0.0055(2)	0.0331(4)	-0.0022(3)	11 F1 9 12 F2		
1223.87237	0.0577(7)	-0.0033(2)	0.0367(4)	-0.0012(2)	10 F1 6 11 F2 3	0.0613(18)	1.0624
1226.84158	0.0572(1)	-0.0021(2)	0.0356(3)	-0.0010(2)	10 F2 7 11 F1 2	0.0597(12)	1.0437
1229.15291	0.0467(14)	-0.0038(16)	0.0279(6)	-0.0009("2)	11 E 6 12 E i	0.0482(16)	1.0321
1229.18032	0.0476(23)	-0.0025(14)	0.0291(6)	-0.0011(2)	11 F2 8 12 F1 1	0.0554(15)	1.1639
1229.23310	0.0518(5)	-0.0026(2)	0.0290(2)	-0.0006(2)	11 A2 3 12 A1 1	0.0521(12)	1.0058
1229.33029	0.0564(9)	-0.0050(5)	0.0342(6)	-0.0022(2)	10 E 5 11 E 1	0.0581(15)	1.0301
1229.70816	0.0573(6)	-0.0028(3)	0.0351(2)	-0.0014(2)	10 F1 7 11 F2 2	0.0596(3)	1.0401
1230.27552	0.0557(5)	-0.0026(1)	0.0337(3)	-0.0011(1)	10 A1 3 11 A2 1	0.0581(11)	1.0431
1230.72523	0.0581(4)	-0.0014(2)	0.0375(3)	-0.0004(2)	9 F1 5 10 F2 3	0.0612(11)	1.0534
1231.43580	0.0409(4)	-0.0028(1)	0.0244(2)	-0.0010(2)	9 E 4 10 E 2	0.0428(10)	1.0465
1232.08734	0.0585(7)	-0.0029(4)	0.0373(3)	-0.0014(2)	9 F2 6 10 F1 2	0.0613(12)	1.0479
1234.22619	0.0583(7)	-0.0024(1)	0.0364(4)	-0.0011(2)	9 A2 3 10 A1 1	0.0605(5)	1.0377
1234.97930	0.0521(5)	-0.0023(1)	0.0310(2)	-0.0007(2)	10 F1 8 11 F2 1	0.0540(9)	1.0365
1235.06119	0.0530(4)	-0.0021(3)	0.0311(3)	-0.0009(2)	10 F2 8 11 F1 1	0.0550(6)	1.0377
1235.83335	0.0590(4)	-0.0027(1)	0.0369(2)	-0.0012(2)	9 F2 7 10 F1 1	0.0614(15)	1.0407
1236.49487	0.0591(6)	-0.0030(2)	0.0362(2)	-0.0014(2)	9 F1 6 10 F2 2	0.0606(10)	1.0254
1238.48642	0.0600(8)	-0.0016(2)	0.0383(4)	-0.0005(2)	8 A1 2 9 A2 1	0.0618(9)	1.0300
1239.00401	0.0595(4)	-0.0002(4)	0.0381(5)	0.0000(2)	8 F1 5 9 F2 2	0.0621(7)	1.0437
1239.54940	0.0603(5)	-0.0038(3)	0.0385(39)	-0.0021(2)	8 F2 5 9 F13	0.0635(7)	1.0531
1240.71353	0.0545(5)	-0.0002(3)	0.0329(5)	0.0002(4)	9 A1 2 10 A2 1	0.0558(8)	1.0239
1240.84479	0.0600(9)	-0.0019(6)	0.0337(5)	-0.0011(2)	9 F1 7 10 F2 1		
1240.90403	0.0554(9)	0.0013(3)	0.0334(4)	-0.0004(3)	9 E 5 10 E 1	0.0563(6)	1.0162
1240.96190	0.0590(7)	-0.0016(15)	0.0382(6)	-0.0016(2)	8 A2 2 9 A1 1	0.0679(14)	1.1508
1242.65722	0.0608(7)	-0.0029(0)	0.0379(4)	-0.0014(1)	8 F2 6 9 F1 2	0.0628(12)	1.0329
1243.01419	0.0584(6)	-0.0030(2)	0.0357(1)	-0.0013(1)	8 E 4 9 E 1	0.0607(14)	1.0394
1246.40830	0.0617(7)	-0.0001(12)	0.0393(11)	-0.0005(4)	7 F1 5 8 F2 2	0.0631(9)	1.0227
1246.55638	0.0581(5)	-0.0034(2)	0.0352(5)	-0.0018(4)	8 F1 6 9 F2 1	0.0586(13)	1.0086
1246.73684	0.0571(5)	-0.0019(8)	0.0347(1)	-0.0014(2)	8 F2 7 9 F1 1	0.0596(7)	1.0438
1246.82159	0.0512(4)	-0.0026(6)	0.0317(1)	-0.0011(2)	7 E 3 8 E 2	0.0520(12)	1.0156
1247.97642	0.0611(4)	-0.0039(2)	0.0391(3)	-0.0019(2)	7 F2 4 8 F1 2	0.0649(8)	1.0622
1249.48460	0.0614(7)	-0.0027(4)	0.0384(3)	-0.0013(2)	7 F1 6 8 F2 1	0.0633(11)	1.0309
1252.31046	0.0590(5)	-0.0026(1)	0.0366(3)	-0.0014(2)	7 E 4 8 E 1	0.0606(7)	1.0271
1252.44005	0.0599(9)	-0.0027(2)	0.0370(3)	-0.0014(2)	7 F2 5 8 F1 1	0.0613(8)	1.0234
1252.65250	0.0588(3)	-0.0015(9)	0.0368(4)	-0.0008(2)	7 A2 2 8 A1 1	0.0620(18)	1.0544
1253.69279	0.0620(8)	-0.0025(1)	0.0396(3)	-0.0010(3)	6 F2 4 7 F1 2	0.0640(11)	1.0323
1254.48868	0.0497(7)	-0.0031(1)	0.0306(3)	-0.0012(2)	6 E 3 7 E 1	0.0517(10)	1.0402
1255.03515	0.0633(6)	-0.0045(4)	0.0410(8)	-0.0021(3)	6 F1 4 7 F22	0.0658(10)	1.0395
1256.07136	0.0620(5)	-0.0030(2)	0.0399(9)	-0.0015(2)	6 A1 2 7 A2 1	0.0637(4)	1.0274
1258.04915	0.0612(9)	-0.0022(1)	0.0391(7)	-0.0005(3)	6 F1 5 7 F2 1	0.0636(5)	1.0392
1258.34756	0.0605(3)	-0.0024(1)	0.0387(5)	-0.0011(2)	6 F2 5 7 F1 1	0.0631(10)	1.0430
1260.54686	0.0629(8)	-0.0024(1)	0.0403(9)	-0.0009(2)	5 A2 2 6 A1 1	0.0645(15)	1.0254
1261.06201	0.0626(6)	-0.0023(10)	0.0405(7)	-0.0005(2)	5 F2 4 6 F1 1	0.0650(11)	1.0383
1261.63748	0.0641(7)	-0.0037(9)	0.0411(10)	-0.0015(4)	5 F1 3 6 F22	0.0661(12)	1.0312

12 ^{g3}	375 ^{g2}	0	0617(11)	-o	o 25(4)	o	o 335	o	0017(- 3)	5	A1 1	6	A2 1	1	0 389
1263	96365	o	0635(8)	-o	o 14(9)	o	o 406(7)	o	o 003(5)	5	F1 4	6	F2 1	1	0 126
1264	13791	o	0608(7)	-o	o 21(6)	o	o 385	o	o 013(2)	5	E 3	6	E 1	1	0 214
1267	59136	o	0633(4)	-o	o 19(1)	o	o 391	16	o 012(11)	4	F2 3	5	F1 2	o	o 657 14)
1267	9165 ^o	o	0577(6)	-o	o 25(1)	o	o 363	3	o 011(2)	4	E 2	5	E 1	o	o 593 12)
1269	31252	o	0620(4)	-o	o 24(25)	o	o 407	6	o 004(13)	4	F1 3	5	F2 1	1	0 277
1269	90994	o	0680(44)	o	o 25(48)	o	o 4 9	1 ^b	o 0013(2)	4	F2 4	5	F1 1	o	o 665 11)
1274	01690	o	0640(4)	-o	o 26(5)	o	o 04(9)	1 ^b	o 010(2)	3	F1 3	4	F2 1	o	o 663 18)
1274	98482	o	0551(7)	-o	o 28(7)	o	o 356(5)	1 ^b	o 017(2)	3	E 2	4	E 1	o	o 0578 13)
1275	32654	o	0648(2)	-o	o 24(1)	o	o 18(6)	1 ^b	o 017(3)	3	F2 2	4	F1 1	o	o 0672 11)
1275	77928	o	0630(5)	-o	o 19(4)	o	o 406	7	o 014(2)	3	A2 1	4	A1 1	o	o 0659 15)
1279	44149	o	0481(6)	-o	o 50(14)	o	o 283	5	o 000(3)	12	A2 1	12	A1 1	o	o 0533(18)
1280	09407	o	0706(42)	-o	o 87(4)	o	o 414	10	o 002(24)	2	A1 1	3	A2 1	1	1 1081
1280	48351	o	0441(14)	-o	o 2 ^w	o	o 278	9	o 016(6)	15	A1 2	15	A2 1	o	o 04 3 4 ^o
1280	70509	o	0648(4)	-o	o 19(3)	o	o 415	8	o 011(2)	2	F1 2	3	F2 1	o	o 386
1281	17699	o	0640(5)	-o	o 34(1)	o	o 411	6	o 022(2)	2	F2 2	3	F1 1	o	o 672 11)
1282	44038	o	0509(6)	-o	o 36(5)	o	o 304	4	o 010(2)	11	F2 3	11	F1 1	o	o 500
1282	47852	o	0521(5)	-o	o 25(7)	o	o 307	3	o 006(2)	11	F1 4	11	F2 1	o	o 432
1283	35465	o	0489(6)	-o	o 24(8)	o	o 290	6	o 008(2)	14	F1 5	14	F2 2	o	o 546 11)
1283	46482	o	0545(7)	-o	o 35(8)	o	o 36(9)	1 ^b	o 032(8)	14	F2 5	14	F1 1	o	o 561(37)
1285	19755	o	0561(10)	-o	o 04(14)	o	o 35(4)	1 ^b	o 005(5)	10	E 2	10	E 1	o	o 0000
1285	23068	o	0533(10)	-o	o 27(6)	o	o 35(5)	1 ^b	o 011(2)	10	F1 3	10	F2 1	o	o 0413
1285	2992 ^b	o	0550(8)	-o	o 030(8)	o	o 328	3	o 003(2)	10	A1 2	10	A2 1	o	o 555(23)
1285	5482	o	0485(44)	-o	o 014(38)	o	o 34(8)	1 ^b	o 0023(16)	13	E 3	13	E 1	o	o 0535 31)
1286	04571	o	0542(5)	-o	o 027(3)	o	o 327	9	o 0012(4)	13	F2 5	13	F1 2	o	o 0569 26)
1286	24332	o	0532(7)	-o	o 15(2)	o	o 327	7	o 0002(2)	13	A2 3	13	A1 1	o	o 0554 19)
1286	51331	o	065 ^b (6)	-o	o 04(18)	o	o 410	8	o 008(3)	1	F1 1	2	F2 1	o	o 672 14)
1286	80353	o	0655(5)	-o	o 22(4)	o	o 405	7	o 014(1)	1	E 1	2	E 1	o	o 670 15)
1287	70323	o	055 ^b	-o	o 22(1)	o	o 34 ^w	5	o 009(2)	9	F2 3	9	F1 1	o	o 371
1287	81607	o	0574(7)	-o	o 021(2)	o	o 31	5	o 006(2)	8	A2 1	8	A1 1	o	o 587 9)
1288	74308	o	0488(43)	-o	o 053(10)	o	o 2 ^c	10	o 021(6)	15	F1 7	15	F2 3	o	o 0307 44)
1289	85802	o	0584(15)	-o	o 1 ^b	o	o 364	1 ^b	o 007(2)	8	A2 1	8	A1 1	o	o 0593 33)
1290	02657	o	0589(4)	-o	o 19(1)	o	o 367	3	o 008(2)	8	F2 3	8	F1 1	o	o 0612(17)
1290	11978	o	0591(8)	-o	o 12(4)	o	o 364	3	o 005(2)	8	E 2	8	E 1	o	o 0595(25)
1290	18290	o	0569(8)	-o	o 25(3)	o	o 335	5	o 009(2)	11	A1 2	11	A2 1	o	o 0668
1290	58222	o	0600(5)	-o	o 70 ^b (3)	o	o 355	6	o 019(10)	11	F1 5	11	F2 2	o	o 0621(60)
1290	8053	o	0579(8)	-o	o 12(3)	o	o 367	6	o 002(2)	11	E 3	11	E 1	o	o 9672
1290	93599	o	0475(8)	-o	o 01 ^b (10)	o	o 306	13	o 007(2)	14	E 4	14	E 2	o	o 583 8)
1291	83197	o	0609(7)	-o	o 14(5)	o	o 383	2	o 004(2)	7	F2 2	7	F1 1	o	o 627 5)
1291	33648	o	0552(1 ^b)	-o	o 39(1 ^b)	o	o 335	2	o 013(3)	13	F2 6	13	F1 3	o	o 0516
1292	15643	o	0608(7)	-o	o 23(12)	o	o 382	2	o 025(10)	7	F2 3	7	F1 1	o	o 378
1292	17299	o	0616(10)	-o	o 3(34)	o	o 402	13	o 022(20)	10	F1 4	10	F2 2	o	o 589 16)
1292	29864	o	0657(10)	-o	o 21(2)	o	o 390	4	o 010(2)	0	F2 1	1	F1 1	o	o 658 16)
1292	71693	o	0601(6)	-o	o 003(13)	o	o 369	6	o 005(2)	10	F2 4	10	F1 1	o	o 283
1292	78152	o	0515(22)	-o	o 0020(10)	o	o 337	9	o 008(2)	13	F1 5	13	F2 2	o	o 0516
1293	04431	o	0402(26)	-o	o 0019(11)	o	o 270(14)	1 ^b	o 010(7)	15	E 15	E 2	E 2	o	o 0796

1293.43242	0.0476	46)	-0.0015	3)	0.0320(4)	-0.0004(2)	12	E	4	12	E	2	0.0564	29)	1.1849
1293.53875	0.0610	8)	-0.0013	9)	0.0388(3)	-0.0008(2)	6	E	2	6	E	1	0.0635	14)	1.0410
1293.66835	0.0592	10)	-0.0018	18)	0.0358(4)	-0.0009(3)	9	E	3	9	E	1	0.0614	17)	1.0372
1293.71632	0.0611	6)	-0.0003	24)	0.0401(7)	-0.0003(4)	6	F1	2	6	F2	1	0.0654	19)	1.0704
1293.88237	0.0576	24)	-0.0005	7)	0.0356(7)	-0.0005(3)	12	F1	5	12	F2	2	0.0591	24)	1.0260
1293.99340	0.0602(22)	-0.0027(25)			0.0377(7)	-0.0004(2)	9	F2	4	9	F1	2	0.0619	14)	2..0282
1294.19642	0.0604(3)	-0.0037(43)			0.0405(12)	-0.0031(15)	6	A1	1	6	A2	1	0.0657	13)	1.0877
1294.60726	0.0564(4)	-0.0004(8)			0.0350(5)	-0.0003(2)	11	F2	4	11	F1	2	0.0585	20)	1.0372
1295.10320	0.0581(21)	0.0003(4)			0.0385(5)	0.0003(3)	9	A2	2	9	A1	1	0.0618	12)	1.0637
1295.30314	0.0566(20)	-0.0015(6)			0.0371(9)	-0.0009(2)	10	AZ	2	10	A1	1	0.0600	14)	1.0601
1295.44917	0.0623(14)	-0.0010(1)			0.0416(8)	0.0000(2)	5	F1	2	5	F2	1	0.0652	15)	1.0465
1295.62643	0.0622(11)	-0.0002(3)			0.0407(10)	0.0003(5"	7	A1	2	7	A2	1	0.0673(44)		1.0820
1295.74709	0.0664(29)	-0.0035(11)			0.0413(7)	-0.0001(16)	4	A2	1	4	A1	1	0.0662(18)		0.9970
1296.03144	0.0606(10)	-0.0005(4)			0.0402(8)	0.0000(3)	8	F2	4	8	F1	2	0.0627(19)		1.0347
1296.24677	0.0635(9)	-0.0008(1)			0.0411(7)	-0.0005(2)	4	F2	2	4	F1	1	0.0673(16)		1.0598
1296.31781	0.0570(20)	-0.0028(1)			0.0382(21)	-0.0046(14	15	A2	2	15	A1	1			
1296.46489	0.0587(36)	0.0000(14)			0.0377(7)	-0.0029(12)	11	F1	6	11	F2	3	0.0602(8)		1.0256
1296.49979	0.0609(22)	-0.0066(21)			0.0418(7)	-0.0042(11)	7	F1	4	7	F2	2	0.0654(14)		1.0739
1296.60044	0.0584(19)	-0.0013(2)			0.0376(9)	-0.0002(3)	4	E	i	4	E	1	0.0594(11)		1.0171
2.296.70106	0.0625(19)	0.0000(12)			0.0412(11)	0.0021(10)	10	F2	5	10	F1	2	0.0608(27)		0.9728
1296.83399	0.0646(16)	0.0000(5)			0.0414(10)	-0.0003(3)	3	F2	1	3	F1	1			
1296.99232	0.0658(5)	-0.0016(13)			0.0433(25)	-0.0001(28)	6	F1	3	6	F2	2			
1297.03222	0.0485(11)	0.0026(11)			0.0310(8)	-0.0001(5)	7	E	2	7	E	1	0.0499(30)		1.0289
1297.13380	0.0591(15)	-0.0018(3)			0.0378(7)	-0.0005(12)	9	F2	5	9	F1	3	0.0627(18")		1.0609
1297.52360	0.0556(34)	-0.0045(9)			0.0370(4)	-0.0015(2)	5	E	2	5	E	1	0.0640(26)		1.1511
1297.68867	0.0287(14)	-0.0026(5)			0.0234(26)	0.0012(5)	13	E	4	13	E	2			
1297.73666	0.0630(25)	0.0010(29)			0.0409(14)	-0.0004(2)	1	F2	1	F1	1				
1297.84345	0.0557(16)	0.0018(32)			0.0404(18)	-0.0005(7)	5	F2	3	5	F1	2	0.0656(35)		1.1957
1297.91412	0.0630(25)	-0.0061(8)			0.0410(26)	-0.0010(3)	4	F1	2	4	F2	1	0.0642(10)		1.0190
1298.29027	0.0644(17)	-0.0002(16)			0.0409(15)	-0.0016(14)	6	A2	1	6	A1	i	0.0663(39)		1.0295
2298.26567	0.0420(16)	0.0099(0)			0.0380(22)	-0.0027(21)	11	F2	5	11	F1	3			
1298.50880	0.0537(47)	-0.0036(15)			0.0366(12)	-0.0029(25)	13	F2	7	13	F1	4			
1298.64544	0.0570(10)	-0.0027(3)			0.0361(5)	-0.0008(7)	12	A2	2	12	A1	2			
1298.93396	0.0516(26)	-0.0023(4)			0.0346(5)	-0.0003(1)	15	A1	3	15	A2	2			
1303.24881	0.0657(8)	-0.0020(1)			0.0406(6)	-0.0007(3)	1	A2	1	0	A1	1	0.0684(8)		1.0411
1308.55131	0.0650(6)	-0.0011(1)			0.0403(5)	-0.0001(2)	2	F2	1	1	F1	1	0.0685(15)		1.0538
1313.72227	0.0648(8)	-0.0016(4)			0.0410(7)	-0.0002(2)	3	F1	1	2	F2	1	0.0680(9)		1.0494
1313.78802	0.0567(17)	-0.0016(5)			0.0354(3)	0.0002(3)	3	E	1	2	E	1	0.0587(7)		1.0353
1318.63518	0.0613(16)	-0.0021(11)			0.0380(1)	0.0000(o)	4	A1	1	3	A2	1	0.0552(. 5)		0.9005
1318.81030	0.0631(7)	0.0006(7)			0.0404(2)	0.0010(o)	4	F1	1	3	F2	1	0.0674(13)		1.0681
1323.56919	0.0629(8)	0.0008(1)			0.0403(5)	0.0007(3)	5	F1	1	4	F2	1	0.0648(6)		1.0302
1323.89528	0.0530(16)	-0.0009(0)			0.0339(3)	0.0001(2)	5	E	1	4	E	1	0.0550(10)		1.0377
2324.01184	0.0639(8)	-0.0022(2)			0.0412(6)	-0.0007(3)	5	F2	1	4	F1	1	0.0662(14)		1.0360
1324.17828	0.0626(10)	-0.0007(4)			0.0395(12)	0.0003(3)	5	A2	1	4	All		0.0633(18)		1.0112
{328.37219	0.0624(5)	-0.0003(5)			0.0402(5)	0.0006(3)	6	F2	1	5	F12		0.0635(21)		1.0176
1328.46747	0.0564(6)	-0.0013(2)			0.0350(6)	-0.0001(3)	6	E	1	5	E1		0.0587(9)		1.0408
1328.98244	0.0627(6)	-0.0024(3)			0.0407(7)	-0.0008(3)	6	F1	1	5	F2	1	0.0654(4)		1.0431

1329.20091	0.0611(6)	-0.0008(1)	0.0392(4)	-0.0001(2)	6	F2 2	5	F1 1	0.0644(18)	1.0540
1329.30913	0.0536(45)	-0.0057(3)	0.0359(7)	-0.0024(3)	6	A12 6	A2 1			
1331.66215	0.0617(7)	-0.0102(92)	0.0415(11)	-0.0043(25)	7	F2 4	7	F1 1		
1332.97040	0.0624(14)	-0.0003(1)	0.0388(7)	0.0022(22)	7	A2 i	6	Al i	0.0640(19)	1.0256
1333.12085	0.0616(9)	0.0017(12)	0.0402(9)	0.0034(9)	7	F2 1	6	F1 1	0.0653(13)	1.0601
1333.29499	0.0630(8)	-0.0046(5)	0.0407(9)	-0.0028(7)	7	F1 1	6	F2 2	0.0624(22)	0.9905
1333.96394	0.0602(7)	-0.0020(4)	0.0413(19)	-0.0023(6)	7	Al 1	6	A2 1	0.0630(13)	1.0465
1334.17275	0.0601(14)	-0.0027(9)	0.0403(5)	-0.0004(2)	7	F1 2	6	F2 1	0.0640(18)	1.0649
1334.24178	0.0602(9)	-0.0016(5)	0.0374(3)	0.0006(4)	7	E 1	6	E 1	0.0606(15)	1.0066
1335.06689	0.0502(38)	-0.0010(25)	0.0391(4)	-0.0041(15)	8	A22 8	Al 1			
1337.61282	0.0619(8)	0.0013(5)	0.0398(7)	0.0015(11)	8	F2 1	7	F1 2	0.0632(15)	1.0210
1337.84977	0.0497(18)	-0.0010(4)	0.0309(9)	-0.0002(3)	8	E 1	7	E 1	0.0503(17)	1.0121
1338.00796	0.0622(8)	-0.0032(6)	0.0401(4)	-0.0015(3)	8	F1 1	7	F2 2	0.0658(20)	1.0579
1338.31068	0.0620(8)	-0.0018(16)	0.0401(6)	-0.0005(3)	8	Al 1	7	A2 1	0.0641(19)	1.0339
1339.14379	0.0576(15)	-0.0025(3)	0.0456(18)	-0.0011(8)	8	F1 2	7	F2 1	0.0624(10)	1.0833
1339.25860	0.0592(6)	-0.0011(2)	0.0370(3)	-0.0005(2)	8	F2 2	7	F1 1	0.0624(13)	1.0541
1342.13812	0.0582(7)	0.0023(13)	0.0379(8)	0.0013(2)	9	F1 1	8	F2 2	0.0622(20)	1.0687
1342.24124	0.0510(9)	-0.0014(2)	0.0317(9)	-0.0001(2)	9	E 1	8	E 2	0.0519(6)	1.0176
1342.59095	0.0621(8)	-0.0031(10)	0.0396(7)	-0.0016(2)	9	F2 1	8	F1 2	0.0628(11)	1.0113
1344.16843	0.0569(38)	-0.0016(29)	0.0359(5)	-0.0010(2)	9	E 2	8	E 1	0.0612(11)	1.1047
1344.21535	0.0575(13)	-0.0012(3)	0.0366(10)	-0.0002(2)	9	F2 2	8	F1 1	0.0588(32)	1.0226
1344.29582	0.0575(10)	-0.0009(3)	0.0359(2)	0.0003(3)	9	A2 1	8	Al 1	0.0600(4)	1.0435
1346.50861	0.0582(4)	0.0008(8)	0.0377(7)	0.0023(8)	10	Al 1	9	A2 1	0.0602(13)	1.0344
1346.63354	0.0653(29)	0.0054(10)	0.0388(9)	0.0027(4)	10	F1 1	9	F2 2	0.0656(16)	1.0046
1346.79462	0.0602(24)	-0.0085(12)	0.0369(3)	-0.0031(5)	10	F2 1	9	F1 3	0.0636(11)	1.0565
1347.19515	0.0591(5)	-0.0057(29)	0.0383(7)	-0.0021(6)	10	A2 1	9	Al 1	0.0617(9)	1.0440
1347.6'1416	0.0596(7)	-0.0015(1)	0.0375(5)	-0.0005(2)	10	F2 2	9	F1 2	0.0622(12)	1.0436
1347.72089	0.0562(12)	-0.0012(3)	0.0348(4)	0.0000(3)	10	E 1	9	E 10	0.0591(11)	1.0516
1349.17053	0.0571(6)	-0.0012(1)	0.0345(4)	-0.0007(2)	10	F1 2	9	F2 1	0.0608(14)	1.0648
1349.23348	0.0565(8)	-0.0008(2)	0.0342(3)	-0.0004(2)	10	F2 3	9	F1 1	0.0587(17)	1.0389
1350.92905	0.0565(8)	0.0037(19)	0.0369(7)	0.0023(*A1)	11	F1 1	10	F2 3	0.0609(11)	1.0779
1351.10077	0.0399(3)	-0.0011(2)	0.0236(3)	0.0002(2)	11	E 1	10	E 2	0.0429(3)	1.0752
1351.25322	0.0582(7)	-0.0045(7)	0.0370(4)	-0.0024(3)	11	F2 1	10	F1 2	0.0602(15)	1.0344
1351.70151	0.0580(8)	-0.0013(1)	0.0356(2)	-0.0003(3)	11	A2 1	10	Al 1	0.0596(13)	1.0276
1352.23197	0.0592(6)	-0.0015(1)	0.0367(3)	-0.0002(2)	11	F2 2	10	F1 1	0.0621(16)	1.0490
1352.41904	0.0573(7)	-0.0018(1)	0.0349(3)	-0.0005(2)	11	F1 2	10	F2 2	0.0585(9)	1.0209
1354.12533	0.0548(9)	-0.0008(9)	0.0326(4)	-0.0002(3)	11	Al 1	10	A2 1		
1354.16793	0.0548(27)	-0.0015(16)	0.0331(6)	0.0016(8)	11	F1 3	10	F2 1		
1354.18778	0.0525(25)	0.0037(33)	0.0318(8)	0.0011(5)	11	E 2	10	E 1		
1355.25149	0.0551(23)	0.0021(5)	0.0371(6)	0.0013(2)	12	F2 1	11	F1 3	0.0575(15)	1.0436
1355.34640	0.0427(15)	-0.0013(1)	0.0262(9)	0.0003(3)	12	E 1	11	E 2	0.0443(11)	1.0375
1355.57918	0.0562(17)	-0.0063(14)	0.0354(6)	-0.0021(4)	12	F1 1	11	F2 3	0.0587(8)	1.0445
1356.15218	0.0562(6)	-0.0013(O)	0.0346(5)	-0.0002(2)	12	F2 2	11	F1 2	0.0587(11)	1.0445
1356.94152	0.0552(3)	-0.0015(4)	0.0333(4)	-0.0007(3)	12	E 2	11	E 1	0.0575(11)	1.0417
1357.03528	0.0567(2)	-0.0016(3)	0.0348(4)	-0.0007(3)	12	F1 2	11	F2 2	0.0584(13)	1.0300
1357.18403	0.0557(6)	-0.0026(2)	0.0334(5)	-0.0006(3)	12	Al 1	11	A2 1	0.0573(11)	1.0287
1359.09573	0.0528(6)	-0.0013(4)	0.0311(4)	-0.0004(3)	12	F1 3	11	F2 1	0.0529(8)	1.0019

1359.12118	0.0503	8)	0.0003(12)	0.0302(3)	-0.0004(2)	12 F2 3 11 F1 1	0.0529(14)	1.0517
1359.45115	0.0533	10)	0.0013(-3)	0.0352(5)	0.0015(-2)	13 A2 1 12 A1 2	0.9561(17)	1.0525
1359.55999	0.0573	11)	0.0060(-7)	0.0366(6)	0.0044(-5)	13 F2 1 12 F1 3	0.0656(11)	1.1449
1359.68908	0.0520	4)	-0.0089(14)	0.0344(7)	-0.0044(-4)	13 F1 1 12 F2 3	0.0615(45)	1.1827
1359.93089	0.0542	6)	-0.0046(-4)	0.0347(5)	-0.0023(-2)	13 A1 1 12 A2 1	0.0567(15)	1 . 0 4 6 1
1360.52019	0.0551(9)	-0.0017(-3)	0.0342(5)	-0.0005(-2)	13 F1 2 12 F2 2	0.0567(-3)	1.0290	
1360.63994	0.0527(8)	-0.0030(-3)	0.0320(9)	-0.0013(-2)	13 E 1 12 E 2	0.0527(10)	1.0000	
1361.64865	0.0546(8)	-0.0012(-5)	0.0331(5)	-0.0007(-1)	13 F2 2 12 F1 2	0.0562(21)	1.0293	
1361.78493	0.0523(8)	0.0000(14)	0.0322(6)	0.0007(-5)	13 F1 3 12 F2 1	0.0551(16)	1.0535	
1363.83988	0.0312(16)	-0.0014(-7)	0.0178(8)	0.0000(-2)	14 E 1 13 E 2			
1363.96201	0.0550(31)	-0.0038(11)	0.0361(-6)	-0.0026(-2)	14 F1 1 13 F2 3	0.0582(-9)	1.0582	
1364.53675	0.0535(7)	-0.0012(4)	0.0330(-2)	-0.0003(2)	14 A1 1 13 A2 1	0.0525(19)	0.9813	
1364.89803	0.0543(6)	-0.0007(2)	0.0331(-6)	-0.0001(2)	14 F1 2 13 F2 2	0.0510(18)	0.9392	
1365.10593	0.0538(6)	-0.0019(5)	0.0333(-7)	-0.0006(2)	14 F2 2 13 F1 3	0.0536(25)	0.9963	
1366.29129	0.0534(4)	-0.0024(3)	0.0320(-3)	-0.0008(1)	14 A2 1 13 A1 1	0.0526(26)	0.9850	
1366.39032	0.0519(4)	-0.0014(4)	0.0312(4)	-0.0003(3)	14 F2 3 13 F1 2	0.0529(40)	1.0193	
1366.43259	0.0497(18)	-0.0005(11)	0.0299(5)	-0.0008(2)	14 E 2 13 E 1	0.0498(31)	1.0020	
1367.89652	0.0508(13)	0.0053 12)	0.0339(8)	0.0040(5)	15 F1 1 14 F2 4			
1367.97470	0.0333(18)	-0.0025(1)	0.0196(7)	0.0001(3)	15 E 1 14 E 3			
1368.12848	0.0502(15)	-0.0065(5)	0.0352(9)	-0.0034(8)	15 F2 1 14 F1 3			
1368.81057	0.0489(16)	-0.0019(11)	0.0322(6)	0.0006(20)	15 F1 2 14 F2 3			
1359.35437	0.0503(24)	-0.0006(4)	0.0284(12)	-0.0001(5)	15 E 2 14 E 2			
1369.48645	0.0549(10)	-0.0021(11)	0.0321(8)	-0.0002(3)	15 F2 2 14 F1 2			
1369.67899	0.0496(7)	-0.0021(3)	0.0289(4)	-0.0003(2)	15 A2 1 14 A1 1	0.0532(12)	1.0726	
1371.01149	0.0538(15)	-0.0005(5)	0.0329(10)	0.0003(1)	15 F2 2 14 F1 1			
1371.06845	0.0517(16)	-0.0030(7)	0.0312(12)	-0.0012(3)	15 F1 3 14 F2 2			
1371.99545	0.0487(14)	0.0026(6)	0.0322(6)	0.0024(5)	16 A1 1 15 A2 2			
1372.07080	0.0597(18)	0.0130(14)	0.0388(4)	0.0078(6)	16 F1 1 15 F2 4			
1372.31988	0.0501(6)	-0.0086(13)	0.0328(5)	-0.0032(3)	16 A2 1 15 A1 1			
1373.0053:	0.0432(8)	0.0003(21)	0.0309(9)	0.0004(7)	16 F2 2 15 F1 3			
1373.12249	0.0394(37)	-0.0008(17)	0.0248(13)	-0.0003(7)	15 E 1 15 E 2			



Frequency (cm^{-1})

figure 1a

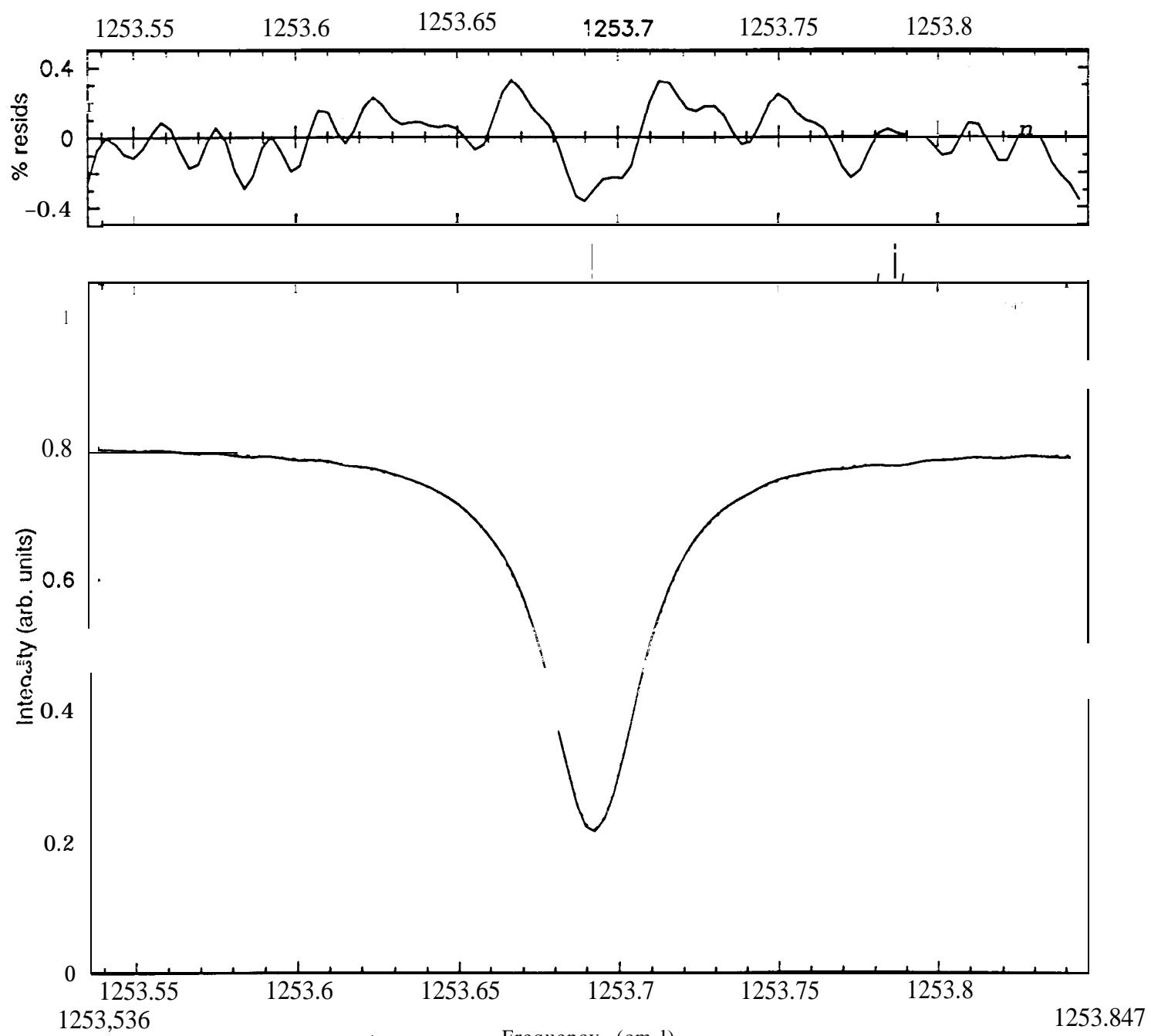


figure 1 b

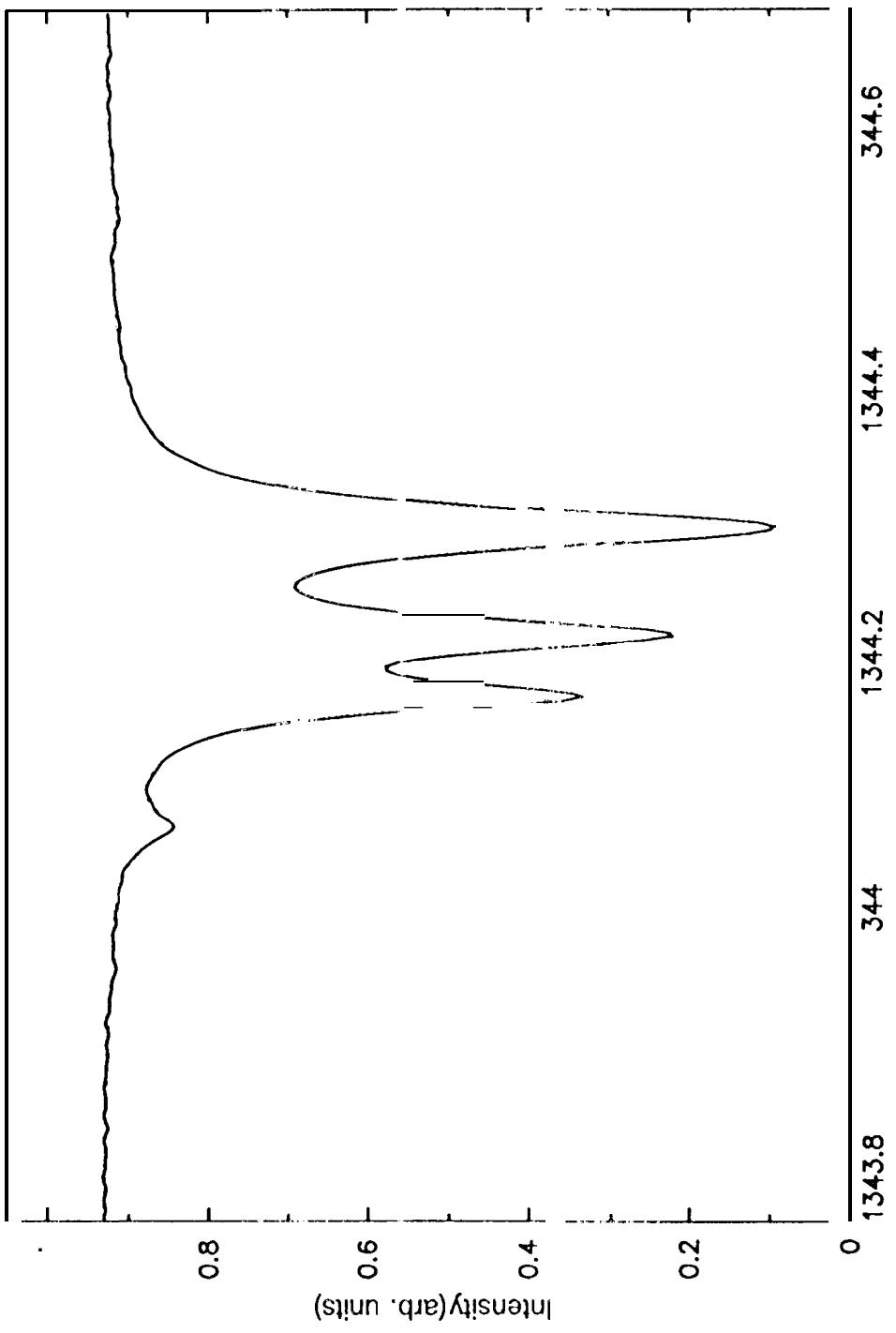
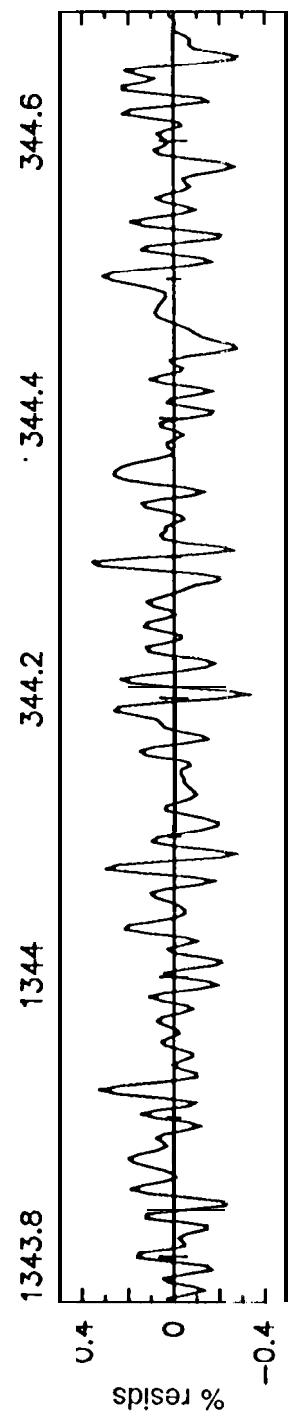


figure 2a

figure 2a

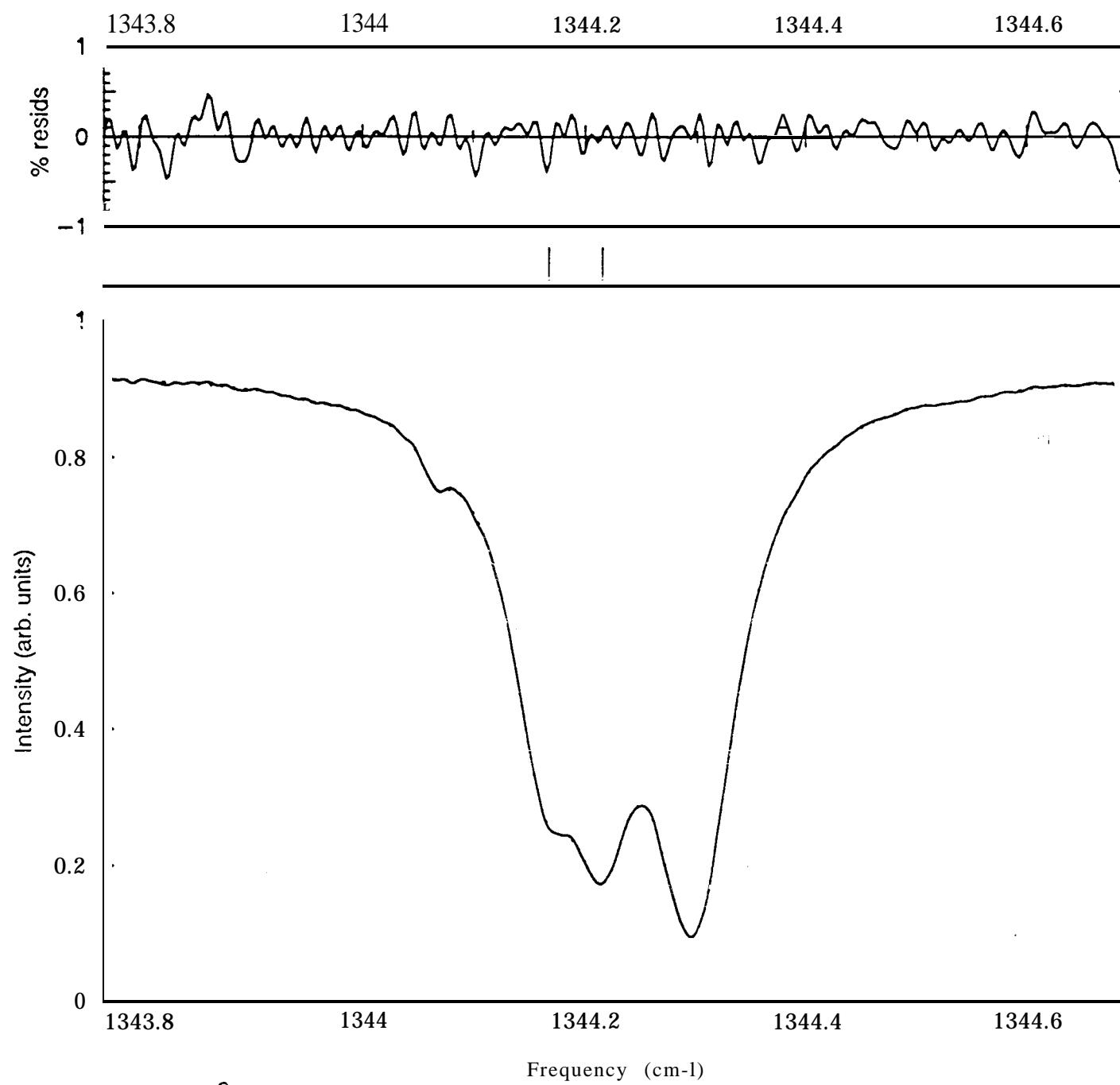
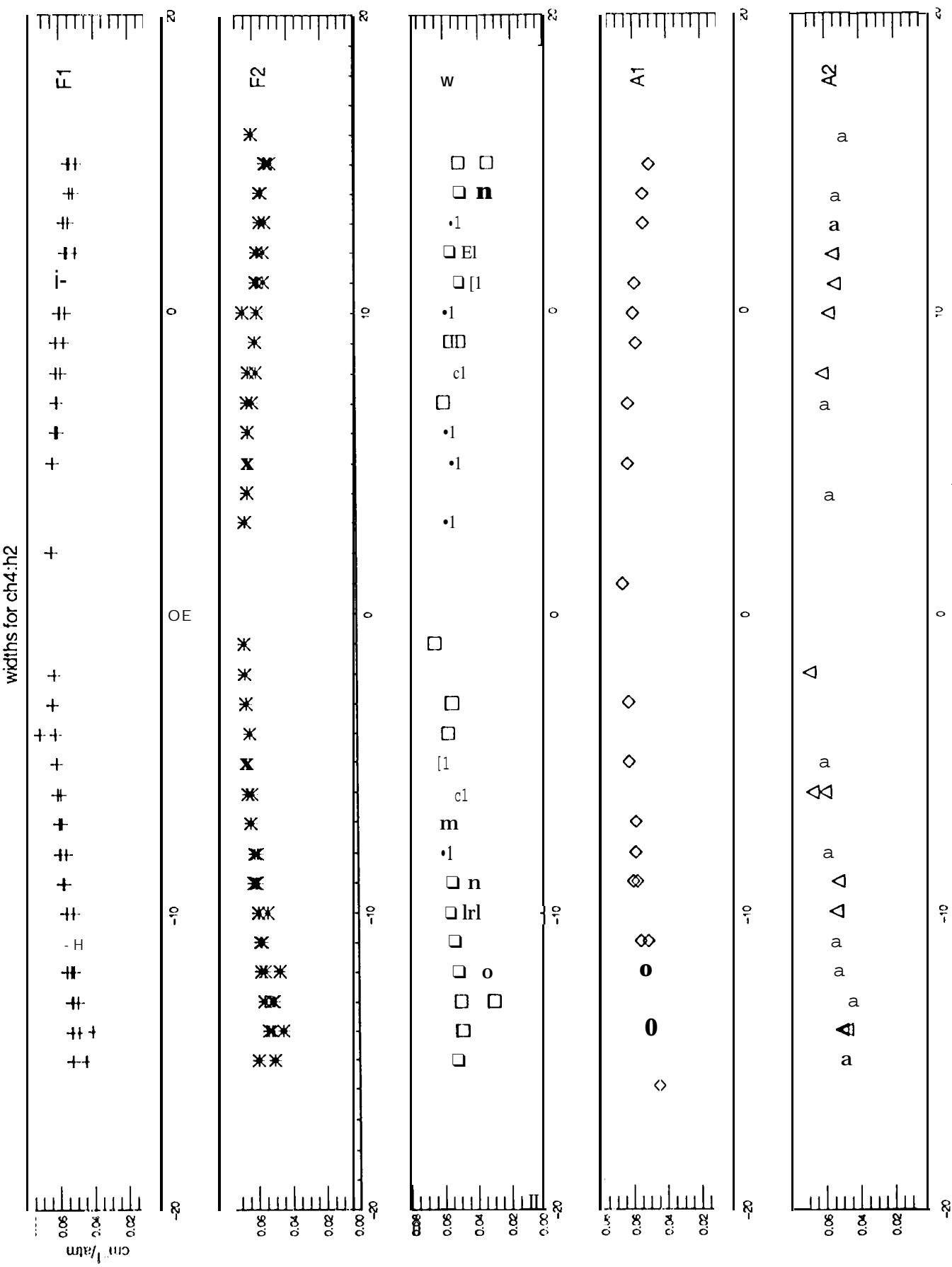


figure 2b

figur 3a



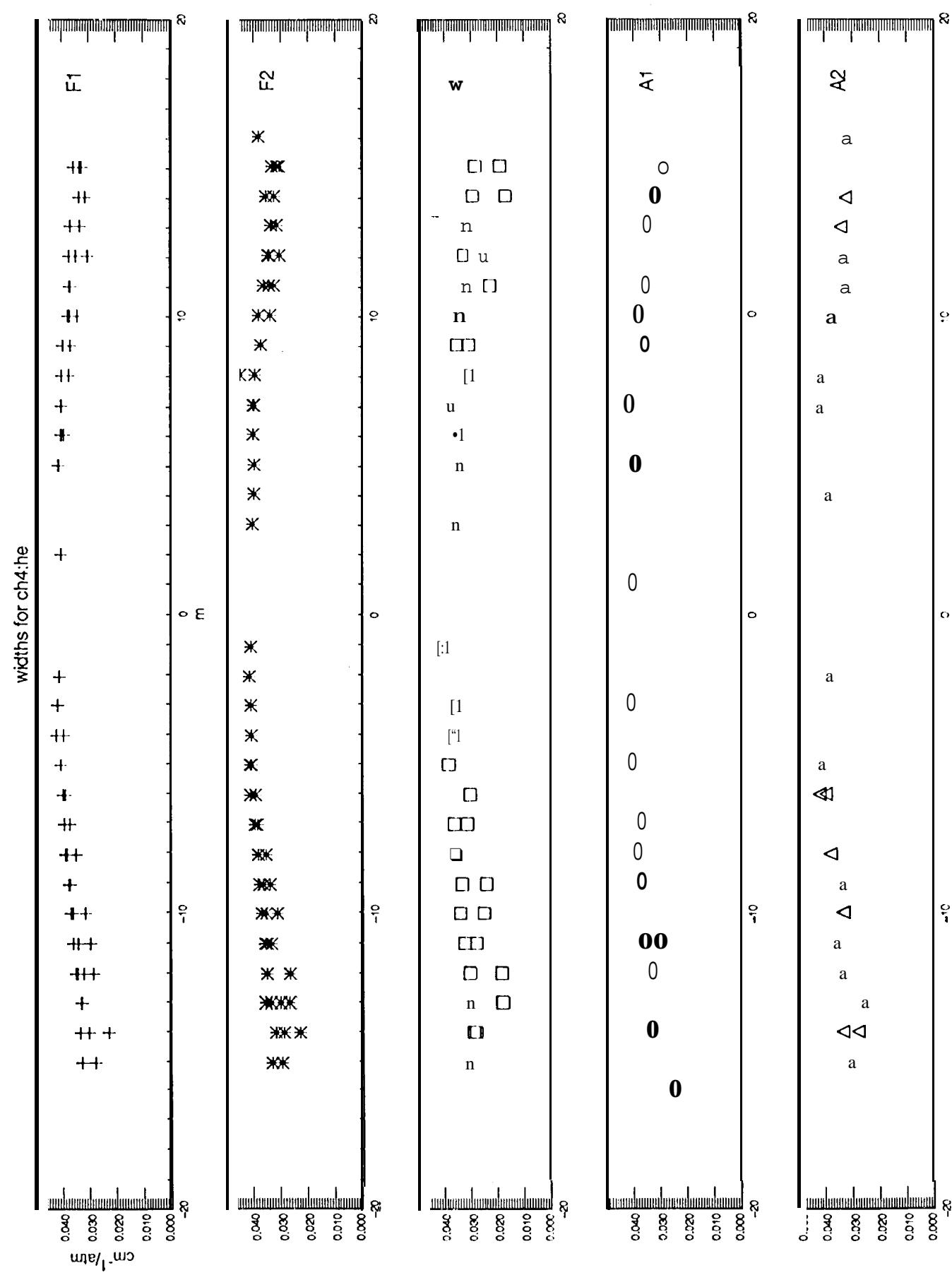


Figure 3b